MDF: Magnetic Particle Imaging Data Format

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Abstract

Magnetic particle imaging (MPI) is a tomographic method to determine the spatio-temporal distribution of magnetic nanoparticles. In this document, a file format for the standardized storage of MPI and magnetic particle spectroscopy (MPS) data is introduced. The aim of the Magnetic Particle Imaging Data Format (MDF) is to provide a coherent way of exchanging MPI and MPS data acquired with different devices worldwide. The focus of the MDF is on sequence parameters, measurement data, calibration data, and reconstruction data. The format is based on the hierarchical document format in version 5 (HDF5). This document discusses the MDF version 2.0.0-pre, which is not backward compatible with version 1.x.y.

1 Introduction

The purpose of this document is to introduce a file format for exchanging Magnetic Particle Imaging (MPI) and Magnetic Particle Spectroscopy (MPS) data. The Magnetic Particle Imaging Data Format (MDF) is based on the hierarchical document format (HDF) in version 5 [1]. HDF5 is able to store multiple datasets within a single file providing a powerful and flexible data container. To allow an easy exchange of MPI data, one has to specify a naming scheme within HDF5 files which is the purpose of this document. In order to create and access

HDF5 data, an Open Source C library is available that provides dynamic access from most programming languages. MATLAB supports HDF5 by its functions h5read and h5write. For Python, the h5py package exists, and the Julia programming language provides access to HDF5 files via the HDF5 package. For languages based on the .NET framework, the HDF5DotNet library is available.

The MDF is mainly focused on storing measurement data, calibration data, or reconstruction data together with the corresponding sequence parameters and metadata. Even though it is possible to combine measurement data and recon-

struction data into a single file, it is recommended to use a single file for each 1.2 of the following dataset types:

- 1. Measurement data
- 2. Calibration data
- 3. Reconstruction data

1.1 Datatypes & Storage Order

MPI parameters are stored as regular *HDF5 datasets*. *HDF5 attributes* are not used in the current specification of the MDF. For most datasets, a fixed datatype is used, for example the drive-field amplitudes are stored as H5T_NATIVE_DOUBLE values. Whenever a data type has a big- and little-endian version, the little-endian data type should be used. For our convenience, we refer to the HDF5 datatypes H5T_STRING, H5T_NATIVE_DOUBLE, and H5T_NATIVE_INT64 as String, Float64 and Int64. Boolean data is stored as H5T_NATIVE_INT8, which we refer to as Int8.

The datatype of the MPI measurement and calibration data offers more freedom and is denoted by Number, which can be any of the following HDF5 data types: H5T_NATIVE_FLOAT, H5T_NATIVE_DOUBLE, H5T_NATIVE_INT8, H5T_NATIVE_INT16, H5T_NATIVE_INT32, and H5T_NATIVE_INT64.

For later identification of a data set, we store three Universally Unique Identifiers (UUIDs) (RFC 4122) [2] in its canonical textual representation as 32 hexadecimal digits, displayed in five groups separated by hyphens 8-4-4-4-12 as for example ee94cb6d-febf-47d9-bec9-e3afa59bfaf8. For the generation of the UUIDs, we recommend to use version 4 of the UUID specification.

Whenever multidimensional data is stored dimensions are arranged in a way that cache is utilized best for fast reconstruction or fast frame selection for example. The leading dimension in the MDF specification is slowest to access and the last dimension is the fastest to access (contiguous memory access). That also means that dependent on the memory lay out of your programming language the order of the dimensions will be just as in the MDF specifications (row major) or reversed (col major). Please take this into account when reading or writing MDF files, which includes the usage of HDF5 viewers.

Since storing complex data in HDF5 is not standardized, we extend the dimensionality of an existing array and store the real and imaginary part in the last dimension with size 2 (index 0 = real part, index 1 = imaginary part). In this way, the real and imaginary part of a complex datum is stored sequentially.

1.2 Units

With one exception, physical quantities are given in SI units. The magnetic field strength is reported in $T\mu_0^{-1} = 4\pi A m^{-1}\mu_0^{-1}$. This convention has been proposed in the first MPI publication [3] and consistently been used in most MPI related publications. The aims of this convention are to report the numbers on a Tesla scale, which most readers with a background in magnetic resonance imaging are familiar with.

1.3 Optional Parameters

The MDF has 8 main groups in the root directory and 2 sub-groups. We distinguish between optional and non-optional groups as well as optional, non-optional, and conditional parameters.

Any optional parameter can be omitted, whereas any non-optional parameter in a non-optional group is mandatory. Conditional parameters are linked to Boolean parameters and have to be provided, if these parameters are true and can be omitted if they are false. If a parameter is optional, non-optional, or conditional is indicated by yes, no, or the corresponding Boolean parameter.

If a group is optional all of its parameters may be omitted, if this group is not used. The groups /, /study, /experiment, /scanner, /acquisition contain mostly metadata and are mandatory. The /tracer group is only mandatory if magnetic material has been placed in the MPI system. The groups /measurement, /calibration, and /reconstruction are all optional. In case of calibration measurements, the /calibration group is mandatory. The reconstruction data is stored in /reconstruction.

1.4 Parameter Extension

Occasionally, it is necessary to store additional specific parameters or metadata that are not covered in the specifications, such as the temperature of the room in which your MPI device is operated. In this case, you are free to add new parameters to any of the existing groups. Moreover, if necessary, you are also free to introduce new groups. In order to be able to distinguish these datasets and groups from the specified ones, we recommend to use the prefix "_" for all parameters and groups. As an example, one could add a new group /_room that includes the dataset _temperature.

1.5 Naming Convention

Several parameters within the MDF are linked in dimensionality. We use short variable names to indicate these connections. The following table describes the meaning of each variable name used.

| Variable | Number of |
|----------------|---|
| \overline{A} | tracer materials/injections for multi-color MPI |
| | |
| N | acquired frames, same as a spatial position for calibration |
| O | acquired frames w/o background frames |
| J | focus-field patches |
| | |
| C | receive channels |
| D | drive-field channels |
| \overline{F} | frequencies describing the drive-field waveform |
| \overline{U} | sampling points describing a custom drive-field waveform |
| | |
| V | points sampled at receiver during one patch (product of drive |
| | field period, number of periods, and number of averages) |
| \overline{W} | sampling points containing processed data ($W = V$ if no fre- |
| | quency selection or bandwidth reduction has been applied) |
| K | frequencies describing the processed data $(K = V/2 + 1)$ if no |
| | frequency selection or bandwidth reduction has been applied) |
| | |
| Q | frames in the reconstructed MPI data set |
| \overline{P} | voxels in the reconstructed MPI data set |
| S | channels in the reconstructed MPI data set |
| | |

1.6 Contact

If you find mistakes in this document or the specified file format or if you want to discuss extensions or improvements to this specification, please open an issue on GitHub:

https://github.com/MagneticParticleImaging/MDF

As the file format is versionized it will be possible to extend it for future needs of MPI. The current version discussed in this document is version 2.0.0-pre.

1.7 arXiv

As of version 1.0.1, the most recent release of these specifications can also be also found at:

https://arxiv.org/abs/1602.06072

If you use MDF, please cite us using the arXiv reference, which is also available for download as MDF.bib from GitHub.

1.8 Code examples

- If you want to get a basic impression of how to handle MDF files you can visit the gitub repository of the MDF project:

https://github.com/MagneticParticleImaging/MDF

There you will find the directory example, which contains a code example written in Julia, MATLAB, and Python. More details can be found in the README of the repository.

1.9 Reference Implementation

A reference implementation for a high level MDF access is available at:

https://github.com/MagneticParticleImaging/MPIFiles.jl MPIFiles.jl is a package written in the programming language Julia [4, 5, 6]. It can read MDF V1, MDF V2, and the dataformat of Bruker MPI systems using a common interface. It also provides functions to convert MDF V1 into MDF V2.

2 Data (group: /)

Remarks: Within the root group, the metadata about the file itself is stored. MPI tracer, and the MPI scanner can be provided. The actual data is stored in Within several subgroups, the metadata about the experimental setting, the dedicated groups about measurement data and reconstruction data.

| Parameter | Type | Dim | Unit/Format | Optional | Description |
|-----------|--------|-----|--|----------|--|
| version | String | 1 | 2.0.0-pre | no | Version of the file format |
| uuid | String | 1 | $3170 {\rm fdf 8-f8e1-4cbf-ac73-41520b41f6ee}$ | no | Universally Unique Identifier (RFC 4122) of MDF file |
| time | String | 1 | yyyy-mm-ddThh:mm:ss.ms | no | UTC creation time of MDF data set |

2.1 Study Description (group: /study/, non-optional)

Remarks: A study is supposed to group a series of experiments to support, refute, or validate a hypothesis. The study group should contain name, number, uuid, and description of the study.

| Parameter | Type | \mathbf{Dim} | ${ m Unit/Format}$ | Optional | Description |
|-------------|--------|----------------|--|----------|---|
| name | String | 1 | | no | Name of the study |
| number | Int64 | 1 | | no | Number of the study |
| uuid | String | 1 | $295258 {\rm fe}\hbox{-}{\rm b}650\hbox{-}4 {\rm e}5 {\rm f}\hbox{-}96 {\rm d}\hbox{b}\hbox{-}{\rm b}83 {\rm f}11089 {\rm a}6 {\rm c}$ | no | Universally Unique Identifier (RFC 4122) of study |
| description | String | 1 | | no | Short description of the study |

2.2 Experiment Description (group: /experiment/, non-optional)

Remarks: For each experiment within a study a name, number, uuid, and aged and the flag isSimulation indicating if data has been obtained via simulation have to be provided. Additionally, the name of the subject imlations have to be stored.

| Parameter | \mathbf{Type} | Dim | ${ m Unit/Format}$ | Optional | Description |
|--------------|-----------------|-----|--------------------------------------|----------|--|
| name | String | 1 | | no | Experiment name |
| number | Int64 | 1 | | no | Experiment number within study |
| uuid | String | 1 | f96dbc48-1ebd-44c7-b04d-1b45da054693 | no | Universally Unique Identifier (RFC 4122) of experiment |
| description | String | 1 | | no | Short description of the experiment |
| subject | String | 1 | | no | Name of the subject that was imaged |
| isSimulation | Int8 | 1 | | no | Flag indicating if the data in this file is simulated rather than measured |

2.3 Tracer Parameters (group: /tracer/, optional)

Remarks: The tracer parameter group contains information about the MPI tracers used during the experiment. For each of the A tracers name, batch, vendor, volume, and molar concentration of solute per liter must be provided. Additionally, the time point of injection can be noted.

This version of the MDF can handle two basic scenarios. In the first one, static tracer phantoms are used. In this case, the phantom contains A distinct tracers. For example, these might be particles of different core sizes, mobile or immobilized particles. In this case, injectionTime is not used. In the second

case, A boli (e.g. pulsed boli) are administrated during the measurement, in which case the approximate administration volume, tracer type and time point of injection can be provided. Note that the injection clock recording the injection time should be synchronized with the clock, which provides the starting time of the measurement.

In case of a background measurement with no applied tracers in the scanner, the optional tracer group can be omitted.

| Parameter | \mathbf{Type} | Dim | ${ m Unit/Format}$ | Optional | Description |
|---------------|-----------------|----------------|--|----------|--|
| name | String | A | | no | Name of tracer used in experiment |
| batch | String | A | | no | Batch of tracer |
| vendor | String | A | | no | Name of tracer supplier |
| volume | Float64 | A | L | no | Total volume of applied tracer |
| concentration | Float64 | \overline{A} | $\mathrm{mol}(\mathtt{solute})/\mathrm{L}$ | no | Molar concentration of solute per litre |
| solute | String | \overline{A} | | no | Solute, e.g. Fe |
| injectionTime | String | \overline{A} | yyyy-mm-ddThh:mm:ss.ms | yes | UTC time at which tracer injection started |

2.4 Scanner Parameters (group: /scanner/, non-optional)

Remarks: The scanner parameter group contains information about the MPI scanner used, such as name, manufacturer, boreSize, field topology, facility where the scanner is installed, and the operator.

| Parameter | \mathbf{Type} | \mathbf{Dim} | $\mathbf{Unit}/\mathbf{Format}$ | Optional | Description |
|--------------|-----------------|----------------|---------------------------------|----------|---|
| name | String | 1 | | no | Scanner name |
| facility | String | 1 | | no | Facility where the MPI scanner is installed |
| operator | String | 1 | | no | User who operates the MPI scanner |
| manufacturer | String | 1 | | no | Scanner manufacturer |
| topology | String | 1 | | no | Scanner topology (e.g. FFP, FFL, MPS) |
| boreSize | Float64 | 1 | m | yes | Diameter of the bore |

2.5 Acquisition Parameters (group: /acquisition/, non-optional)

Remarks: The acquisition parameter group can describe different imaging protocols and trajectory settings. The corresponding data is organized into general information, a subgroup containing information on the D excitation channels, and a subgroup containing information on the C receive channels.

In MPI, a frame groups all data used to reconstruct a single MPI image/tomogram. In the simplest scenario, this data is acquired during one /drivefield/period. The acquisition time increases by a factor of

numAverages if averaging is applied and by a factor of numPeriods if data is recorded over several (averaged) cycles. In a multi-patch setting J offsetFields or mechanical movements shift the gradient field by offsetFieldShift, where J is the number of patches numPatches of a multi-patch measurement. For each shift at least one full drive field cycle is used to acquire the measurement data. For instance, a Cartesian 2D trajectory with 100 lines could be realized by setting numPatches = 100.

| Parameter | Type | \mathbf{Dim} | Unit/Format | Optional | Description |
|------------------|---------|----------------|---------------------------|----------|--|
| startTime | String | 1 | yyyy-mm-ddThh:mm:ss.ms | no | UTC start time of MPI measurement |
| framePeriod | Float64 | 1 | S | no | Time to complete a full frame (product of /drivefield/period, numPeriods, numAverages, and numPatches) |
| numPeriods | Int64 | 1 | 1 | no | Number of drive-field periods per patch |
| numAverages | Int64 | 1 | 1 | no | Number of block averages per patch |
| numPatches | Int64 | 1 | 1 | no | Number of patches within a frame denoted by J |
| numFrames | Int64 | 1 | 1 | no | Number of available measurement frames N |
| gradient | Float64 | $J \times 3$ | ${\rm Tm}^{-1}\mu_0^{-1}$ | yes | Gradient strength of the selection field in x, y , and z directions |
| offsetField | Float64 | $J \times 3$ | $T\mu_0^{-1}$ | yes | Offset field applied for each patch in the measurement sequence |
| offsetFieldShift | Float64 | $J \times 3$ | m | yes | Position of the field free point (relative to origin/center) |

2.5.1 Drive Field (group: /acquisition/drivefield/, non-optional)

Remarks: The drive field subgroup describes the excitation details of the imaging protocol. On the lowest level, each MPI scanner contains D channels for excitation. Since most drive-field parameters may change from patch to patch, they have a leading dimension J.

These excitation signals are usually sinusoidal and can be described by D amplitudes (drive field strengths), D phases, a base frequency, and D dividers. In a more general setting, the generated drive field of channel d can be described by

$$H_d(t) = \sum_{l=1}^F A_l \Lambda_l (2\pi f_l t + \varphi_l)$$

where F is the number of frequencies on the channel, A_l is the drive-field strength, ϕ_l is the phase, f_l is the frequency (baseFrequency/divider $_l$), and Λ_l is the waveform. The waveform is specified by a dedicated parameter waveform. It can be set to sine, triangle, or custom. If set to custom, one can specify a custom waveform using the parameter customWaveform. The number of sampling points of the customWaveform is denoted by U. The triangle is defined to be a 2π periodization of the triangle function:

$$\Lambda_{\rm tri}(t) = \left| t + \frac{\pi}{2} \right| - \frac{\pi}{2} \quad \text{with} \quad -\frac{3}{2}\pi \le t \le \frac{\pi}{2}.$$

| Parameter | Type | Dim | ${ m Unit/Format}$ | Optional | Description |
|----------------|---------|---------------------|--------------------|----------|---|
| numChannels | Int64 | 1 | 1 | no | Number of drive field channels, denoted by D |
| strength | Float64 | $J\times D\times F$ | $T\mu_0^{-1}$ | no | Applied drive field strength |
| phase | Float64 | $J\times D\times F$ | rad, $[-\pi,\pi)$ | no | Applied drive field phase φ |
| baseFrequency | Float64 | 1 | Hz | no | Base frequency to derive field frequencies |
| customWaveform | Float64 | $D\times F\times U$ | 1 | yes | Custom waveform table |
| divider | Int64 | $D \times F$ | 1 | no | Divider of the baseFrequency to determine the drive field frequencies |
| waveform | String | $D \times F$ | 1 | no | Waveform type: sine, triangle or custom |
| period | Float64 | 1 | S | no | Trajectory period is determined by lcm(divider)/baseFrequency |

2.5.2 Receiver (group: /acquisition/receiver/, non-optional)

Remarks: The receiver subgroup describes the details on the MPI receiver. For a multi-patch sequence, it is assumed, that the signal acquisition only takes place during particle excitation. During each drive-field cycle, C receive channels record some quantity related to the magnetization dynamic. In most cases these, will be a continuous voltage signals induced into the C receive coils, which are proportional to the change of the particle magnetization. This analog signal will usually be converted by some sort of analog to digital converter (ADC) to a discrete series of integer numbers r_{ci} for each channel c. To map the these values to the MPI measurement signal u_{ci}^{ADC} , one has to scale the numbers r_{ci} and add an offset factor

$$u_{ci}^{ADC} = a_c r_{ci} + b_c.$$

Here, a_c and b_c are the scaling and offset factors corresponding to channel c, which can be stored in dataConversionFactor. In case the conversion was already performed the dataConversionFactor can be ommitted.

The MPI measurement signal is acquired at V equidistant time points. For inductive measurement systems the signal is usually not measured directly at the receive coils but amplified and filtered first, which may damp and distort the signal. Therefore, a transfer function can be stored in the parameter

transfer Function, which relates the Fourier domain voltage induced at the receive coil $\hat{u}_k^{\rm coil}$ and the Fourier domain voltage $\hat{u}_k^{\rm ADC}$ measured at the ADC by

$$\hat{u}_k^{\text{ADC}} = a_k \hat{u}_k^{\text{coil}}, \quad k = 1, \dots, K.$$

Here, a_k are the unitless parameters stored in transferFunction for each receive channel individually.

For MPS systems one can additionally store a parameter that maps the induced voltage to the magnetic moment of a magnetic nanoparticle located at the center of the scanner. More precisely, in each receive coil a projection of the magnetic moment onto the coil sensitivity is measured. The relation of this projection and the voltage at the receive coil in frequency space representation is given by

$$\hat{u}_k^{\text{coil}} = 2\pi i k \beta \hat{m}_k^{\text{proj}}, \quad k = 1, \dots, K.$$

where \hat{m}_k^{proj} is the orthogonal projection of the full magnetic moment at the scanner center and β is the channel dependent conversion factor that is stored in the parameter inductionFactor.

| Parameter | \mathbf{Type} | \mathbf{Dim} | $\mathbf{Unit}/\mathbf{Format}$ | Optional | Description |
|----------------------|-----------------|-----------------------|---------------------------------|----------|--|
| numChannels | Int64 | 1 | | no | Number of receive channels C |
| bandwidth | Float64 | 1 | $_{ m Hz}$ | no | Bandwidth of the receiver unit |
| numSamplingPoints | Int64 | 1 | | no | Number of sampling points during one patch, denoted by V |
| unit | String | 1 | | no | SI unit of the measured quantity, usually Voltage V |
| dataConversionFactor | Float64 | $C \times 2$ | unit | yes | Dimension less scaling factor and offset (a_c, b_c) to convert raw data into a physical quantity with corresponding unit of measurement unit |
| transferFunction | Float64 | $C \times K \times 2$ | | yes | Transfer function of the receive channels in Fourier domain. unit is the field from the /measurement group |
| inductionFactor | Float64 | C | unit $\mathrm{A^{-1}m^{-2}}$ | yes | Induction factor mapping the projection of the magnetic moment to the voltage in the receive coil. |

2.6 Measurement (group: /measurement/, optional)

Remarks: MPI data is usually acquired by a series of measurements and optional background measurements. Here, we refer to background measurements as MPI data captured, when any signal generating material, e.g. a phantom or a delta sample is removed from the scanner bore. Initially, all data is available in time domain, where the data of a single frame consists of the signal recorded for all patches in each receive channel, i.e. $J \times C \times V$ data points per set with the temporal index being the fastest to access. If several measurements are acquired (indicated by numFrames), the frame dimension is the slowest to access. Along this dimension, the frames are ordered with respect to the time at which they were acquired starting with the measurement acquired first and stopping with the measurement acquired last. We refer to this data as raw measurement data. In Fourier representation, each frame would be stored by $J \times C \times K \times 2$ data points with the last dimension accounting for the complex data and K = V/2 + 1.

Often it is not convenient to store the raw data but to perform certain processing steps and store the processed data. These steps may lead to a reduction of the number of sampling points from V to W or a corresponding reduction of frequency components K depending on the final representation in which the raw/processed data is stored. The most common processing steps are:

1. Spectral leakage correction, which may be applied to ensure that each individual frame is periodic.

- 2. Background correction, where the background signal in subtracted.
- 3. Fourier transformation bringing the data from time into the Fourier representation an storing them in Fourier representation.
- 4. Transfer function correction to obtain the magnetic moment or induced voltage that has been measured.
- 5. Frequency selection to reduce the number of frequency components, e.g. bandwidth reduction or selection of high signal frequency components.
- 6. Dimension permutation, which is usually applied to Fourier transformed data exchanging the storing order of the data for fast access to the frames.
- 7. Frame permutation to reorder the frames within the data set.

For each of the steps above there is a corresponding flag within this group indicating if the corresponding processing step has been carried out.

During processing one might want to keep track which of the final N frames belong to background measurements and which do not. Therefore, the binary mask <code>isBackgroundFrame</code> can be used. If <code>isBackgroundFrame</code> is not provided,

it is assumed that no background measurements are present. If frequency se- $\sigma:\{1,2,\ldots,N\} \to \{1,2,\ldots,N\}$ of the set of frame indices to itself. If such a ponents (subset) selected from the set of acquired frequency components. If $\sigma(N)$ in framePermutation. performed, a frame permutation can be described by i.e. a bijective mapping

lection has been performed, frequencySelection stores the K frequency compermutation is performed, σ is stored in the one-line notation as $\sigma(1)$, $\sigma(2)$, ...,

| Parameter | \mathbf{Type} | Dim | Optional | Description |
|--|-----------------|--|----------------------|--|
| data | Number | $N \times J \times C \times K \times 2$ or $J \times C \times K \times N \times 2$ or $N \times J \times C \times W$ or $J \times C \times W \times N$ | no | Processed data |
| isBackgroundFrame | Int8 | N | yes | Mask indicating for each of the N frames if it is a background measurement (true) or not |
| isSpectralLeakageCorrected | Int8 | 1 | no | Flag, if spectral leakage correction has been applied |
| isBackgroundCorrected | Int8 | 1 | no | Flag, if the background has been subtracted |
| isFourierTransformed | Int8 | 1 | no | Flag, if the data is stored in frequency space |
| $\verb isTransferFunctionCorrected \\$ | Int8 | 1 | no | Flag, if the data has been corrected by the transferFunction |
| isFrequencySelection | Int8 | 1 | no | Flag, if only a subset of frequencies has been selected and stored, see frequencySelection |
| isPermuted | Int8 | 1 | no | Flag, if the frame dimension N has been moved to the last dimension (second last for complex data) |
| isFramePermution | Int8 | 1 | no | Flag, if the order of frames has been changed, see framePermutation |
| frequencySelection | Int64 | K | isFrequencySelection | Indices of selected frequency components |
| framePermutation | Int64 | N | isFramePermutation | Indices of original frame order |

2.7 Calibration (group: /calibration/, optional)

Remarks: The calibration group describes a calibration measurement (system matrix), although it does not hold the data itself. Each of the measurements is taken with a calibration sample (delta sample) at a fixed position inside the FOV of the device. (If available, the background measurements are taken with the delta sample outside of the FOV of the scanner.) Usually, the calibration measurements are not stored as raw measurements but as processed data, where at least averaging, Fourier transformation, frame permutation and transposition of the data has been performed yielding N processed calibration frames. N includes the background measurements, whereas O is the number of calibrated spatial positions scans. Which steps have been performed is documented in /measurement.

If the measurements were taken on a regular grid of size $N_x \times N_y \times N_z$, the permutation is usually done such that measurements are ordered with respect to their x position first, second with respect to their y position, and last with respect to their z position. Background measurements are collected at at the end in /measurement/data, which in combination with reordering of the measurements allows a fast access to the system matrix. If a different storage order is used this can be documented using the optional parameter order. For non-regular sampling points, there is the possibility to explicitly store all O positions. In case of acquiring a hybrid system matrix, the spatial positions may be emulated by applying offsetFields to the measurement chamber.

| Parameter | Type | Dim | Unit/Format | Optional | Description |
|-------------------|---------|---------------------|---------------|----------|--|
| method | String | 1 | | no | Method used to obtain calibration data. Can for instance be robot, hybrid, or simulation |
| size | Int64 | 3 | | yes | Number of voxels in each dimension, inner product is O |
| order | String | 1 | | yes | Ordering of the dimensions, default is xyz |
| positions | Float64 | $O \times 3$ | m | yes | Position of each of the grid points, stored as (x, y, z) triples |
| offsetFields | Float64 | $O \times 3$ | $T\mu_0^{-1}$ | yes | Applied offset field strength to emulate a spatial position (x, y, z) |
| deltaSampleSize | Float64 | 3 | m | yes | Size of the delta sample used for calibration scan |
| fieldOfView | Float64 | 3 | m | yes | Field of view of the system matrix |
| fieldOfViewCenter | Float64 | 3 | m | yes | Center of the system matrix (relative to origin/center) |
| snr | Float64 | $J\times C\times K$ | | yes | Signal-to-noise estimate for recorded frequency components |

2.8 Reconstruction Results (group: /reconstruction/, optional)

Reconstruction results are stored using the parameter data inside this group. data contains a $Q \times P \times S$ array, where Q denotes the number of reconstructed frames within the data set, P denotes the number of voxels and S the number of multispectral channels. If no multispectral reconstruction is performed, then one may set S=1. Depending on the reconstruction the grid of the reconstruction data can be different from the system matrix grid. Hence, grid parameters are mirrored in the /reconstruction group.

For analysis of the MPI tomograms, it is often required to know which parts of the reconstructed tomogram have been covered by the trajectory of the field free region. In MPI, one refers to the non-covered region as overscan region. Therefore, the optional field <code>isOverscanRegion</code> indicated for each voxel if it is part of the overscan region. If no voxel lies within the overscan region, <code>isOverscanRegion</code> may be omitted.

| Parameter | \mathbf{Type} | Dim | Unit/Format | Optional | Description |
|-------------------|-----------------|---------------------|-------------|----------|---|
| data | Number | $Q\times P\times S$ | | no | Reconstructed data |
| size | Int64 | 3 | | yes | Number of voxels in each dimension, inner product is P |
| order | String | 1 | | yes | Ordering of the dimensions, default is xyz |
| positions | Float64 | $P \times 3$ | m | yes | Position of each of the grid points, stored as (x, y, z) tripels |
| fieldOfView | Float64 | 3 | m | yes | Field of view of reconstructed data |
| fieldOfViewCenter | Float64 | 3 | m | yes | Center of the reconstructed data (relative to scanner origin/center) |
| isOverscanRegion | Int8 | P | | yes | Mask indicating for each of the P voxels if it is part of the overscan region (true) or not |

3 Changelog

$3.1 \quad v2.0.0$

- Version 2 of the MDF is a major update breaking backwards compatibility with v1.x. The major update was necessary due to several shortcomings in the v1.x.
- The naming of parameters was made more consistent. Furthermore, some parameters move from one group into another.
- In v1.x it was not possible to store background data. This functionality
 has been added in v2.
- We simplified the measurement group and made it much more expressive. In v1.x it was not entirely clear, which processing steps have been applied to the measurement data in the store dataset. The measurement group now contains several flags that precisely describe the state of the stored data. Using this it is now possible to also store calibration data in the measurement group. The calibration group in turn only stores metadata about a calibration experiment while the actual data is store in the measurement group.
- Updated Affiliations in the MDF specification.
- \bullet Improved the general descriptions of fields and groups.
- In v1.x the MDF allowed many fields to have varying dimensions depending on the context. As of version 2.0.0 only one field offers this freedom. This change should make implementations handling MDF files less complex.
- Number has been introduced as generic types. The type restriction for several parameters has been weakened to these types.
- Added a table listing all variable names used in the descriptions of parameters.
- Added a section describing the possibility to add custom fields to MDF files.
- Added a description for optional and non-optional groups and conditional, optional, and non-optional datasets.

- Added a short section on the code examples on the Github repository.
- Support for triangle wave forms and fully arbitrary excitation waveforms has been added.
- Support for multiple excitation frequencies on a drive-field channel has been added.
- Added the dimension A to all fields of the tracer group to be able to describe settings where multiple tracers are used or tracers are administered multiple times.
- Added the possibility to store the tracer concentration also for non iron based tracer materials by adding the /tracer/solute field and redefining the field tracer/concentration.
- Improved documentation for the storage of receive transfer functions. It is also possible now to store the measurement data as integer data and use a dataConversionFactor to describe the mapping to a physical representation (e.g. Volt)
- Split the /study group into the /experiment group and the study group. This allows to provide more fine grained information on study and experiment.
- Added possibility to mark the overscan region.
- Added new section changelog to the MDF documentation to record the development of the MDF.
- Updated README.md in the github repository.
- Updated code examples in the github repository.
- Added a section on the MDF reference implementation MPIFiles.jl. Since sanity checks will be covered by this package, the description on sanity checks has been removed.

3.2 v1.0.5

- Added the possibility to store different channels of reconstructed data.
- Added support for receive channels with different characteristics (e.g. bandwidth).
- Made dataset /acquisition/receiver/frequencies optional.
- Extended the description on the data types, which are used to store data.
- Added references for Julia and HDF5 to the specifications.

3.3 v1.0.4

• Clarify that HDF5 datasets are used to store MPI parameters.

3.4 v1.0.3

- Updated Affiliations in the MDF specification.
- \bullet Included data download into the Python and Matlab example code.

• Changes in the Python and Matlab example code to be better comparable to the Julia example code.

$3.5 \quad v1.0.2$

• Added reference to arXiv paper and bibtex file for reference.

3.6 v1.0.1

- A sanity check within the Julia code shipped alongside the specifications.
- An update to the specification documenting the availability of a sanity check.
- Updated MDF files on https://www.tuhh.de/ibi/research/mpi-data-format.html.
- Updated documentation to the Julia, Matlab and Python reconstruction scripts.
- Improved Julia reconstruction script, automatically downloading the required MDF files.

References

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